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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Characterizing model errors in chemical transport modelling of methane: Using GOSAT XCH_4 data with weak constraint four-dimensional variational data assimilation" *by* Ilya Stanevich et al.

Anonymous Referee #4

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General Review Comments:

This is a significant and important body of work and I believe the community will find it very interesting. The main limitations I see are in terms of the figures which don't always back up the assertions in the text. Sometimes, in the case of Fig6/Fig7, they clearly support the text but seem to fail because of lack of difference plots or poor choice of color scales. The text is sometimes hard to follow because of the multiple terms being used, eg. state/forcings/3D CH4 adjustments and parameters vs. surface fluxes. After providing the theory, it might be wise to work with common terminology.

Furthermore, I particularly found the assumed variability of the "forcings" in time and space, somewhat hard to follow. In summary though, the work is quite interesting and novel in its handling of the main source of error in atmospheric trace gas inversions (transport).

Specific Comments:

caption Figure 2: "and smoothed with the GOSAT averaging kernels" The authors should give the exact equation they use to calculate modeled XCH4 from their model: is the prior CH4 profile assumed in the retrieval used in this calculation, in addition to the averaging kernel, or not?

Figure 6: Fig 7 provides a motivating summary of Fig 6. However, looking at Fig 6 relative to its colorbar, it is hard to see that the two even provide the same information. I'd really consider adopting a more dynamic color palette for this image.

p6 l10: "...with smaller [modeled] XCH4 in the SH..." A difference plot would be helpful in Figure 2. I am having a very hard time seeing how XCH4 is lower in the SH in the model (top panel) than in the measurements (bottom panel) – the opposite appears to be the case, to my eye.

p6 l11: I agree that China, India, and equatorial Africa are higher in the model, but South America appears to be lower, at least over the Amazon. Again, a difference plot in Figure 2 would help.

p7 l29-on: "The 4D-Var problem to estimate surface emissions is transformed into a 3D sources and sinks estimation problem..." I think you ought to be a bit more precise with the wording here. The 4Dvar method in general can be used to estimate both surface sources/sinks and 3D fields, either using the strong- or weak-constraint dynamics. I think what you want to say is that for your application, which in the past was solving only for surface fluxes and not 3D fields, you are now allowing this 3D forcing term to be solved for, as well. You might want to mention here that you are not too concerned with

what this 3D field represents in your application – it could be a chemical source/ sink, a correction to the 3D concentration field, or a dynamical error. That comment would help those who are accustomed to thinking of this term as being solely a dynamical error term in the weak-constraint approach.

p8 L15: There is a spurious extra term in the cost function here that should lead to some "double counting" of the dynamical errors. To be specific, the last two terms in the cost function both involve the dynamical mismatches, while only one is needed, and that term ought to be: ... + [-Gu_i]^T [Q_i]^-1 [-Gu_i] , which equals ... + (x_i - M(x_i-1,p))^T [Q_i]^-1 (x_i - M(x_i-1,p))

If we note that lambda_i = [Q_i]^-1 (x_i - M(x_i-1,p)), then there is no need to carry around the additional variable u_i, and u_i can be calculated from lambda_i as

G u_i = - [Q_i] lambda_i

Similarly, it is not necessary to have equations for the partial of L with respect to both lambda_i and u_i.

p10 L5: "... a priori estimates of the model errors were set to zero." Just to be sure here, you are setting the actual initial model errors themselves equal to zero (u_i=0) and not the assumed uncertainty in those same errors (Q_i=0), correct? Because setting Q_i=0 would be equivalent to reverting back to the hard dynamical constraint. Writing this out with the mathematical symbols would eliminate any uncertainty the reader might have on that score. p10 second paragraph: This discussion of the relative weighting of the forcing versus emission parts of the solved-for control vector points to something that could be simplified in this approach. It can be shown that the forcing vector -Gu_i at any iteration is simply [Q_i] lambda_i – that is, the adjoint state vector times the assumed model error covariance matrix. The forcing vector does not need to be solved for in the control vector – it is already solved for in the strong-constraint 4Dvar, essentially, since lambda_i is solved for. All that needs to be done to implement the weak-constraint version is to add the forcing vector (=[Q_i] lambda_i) onto the

state at each step during the forward runs (although saving lambda_i at fine temporal resolution, at the timestep of the model, for example, can take a lot of memory and I/O time). Once this is recognized, it is clear that the full parameter space of the forcing vector can be solved for, up to the temporal resolution limits just mentioned. Since it is not too clear what the magnitude of [Q_i] ought to be, some experimentation with the relative weighting between the forcing and emissions parts of the cost function is probably still needed, even with the simplification just noted.

p10 L32-34: "Instead, we use the WC 4D-Var method to optimally constrain the CH4 state and explore the nature of the errors in the model CH4 simulation." Actually, you are not really solving for an optimal estimate of the CH4 state (the 3D CH4 field at each timestep), because you have not put this in the control vector that you are solving for. This state evolves according to your model M and has dynamical constraints upon it. What you are really solving for is some sort of error term on the state, which might be thought of as a dynamical error, or a 3D source/sink (e.g. a chemical one) if one is not modeled, or an error on a modeled 3D source/sink. Since the measurements have error on them, this also allows large measurement errors to be given less importance in the problem (the measurement error is turned into a large forcing error and its effect is on the actual parameters solved-for is lessened).

p10 L33-34: "We performed two types of inversions: “full state assimilation” and “flux+state assimilation”." Point back to your description of these two cases in Section 2.3 here. I had already forgotten that you described them earlier by this point. Also, it wouldn’t hurt to say explicitly that the "full state" case solves only (or mainly) for u, while the "flux+state" case solves for both u and p. Spell it out, especially since the state is defined as "x" earlier, and you don’t actually solve for the full 3-D field "x" in your control vector, no? I guess you get the 3D CH4 fields by adding on the dynamical errors that you do solve for onto the state using equation (2), right?

p11 L13: This would be a good place to mention that, in all these OSSEs, the same transport model was used to generate the truth as was used in the inversion. In other

words, these are all "perfect model" experiments in all respects except the isolated error signal looked at in each experiment. This is important to say, because most readers will be thinking of the weak constraint as a way to handle general model errors, and might be thinking that you used a different transport model for the generating the truth and doing the inversion (I will actually advocate adding an OSSE of this sort below in the emissions case.)

p13 L29-31: Isn't the greater sensitivity in the upper troposphere / lower stratosphere also due to the fact that the GOSAT Xch4 averaging kernel is weighted most heavily in the mid- to upper-troposphere (it being a thermal IR measurement)? A small figure showing what the GOSAT XCH4 averaging kernel actually looks like might be valuable here.

p14 L9: "The results confirm that the SC 4D-Var method better removes CH4 biases due to emissions." This is misleading. Yes, in this setup the SC does better than the WC because it puts all the measurement information into the cause of the difference, the emissions, by design (it doesn't solve for the 3D forcing corrections) as you have noted. But in general case of when there are model errors, the WC case should solve for emissions more accurately than the SC case. It would be really useful if you could have done an additional OSSE here in which you introduced emissions errors AND dynamical errors in the truth, then tried to estimate both using the SC case and the WC "flux+state" setup. That ought to show the WC case doing better, since it would correctly partition the dynamical and emissions errors to the forcing terms and emissions parameters, whereas the SC would incorrectly attribute the dynamical errors solely as emissions errors. You should use a completely different transport model in generating the truth from what is used in the inversion to make this case realistic. The dynamical errors in Q should be based on the differences between the two transport models. I think that that new OSSE would demonstrate the benefit of the WC approach for that case that a lot of readers care about: how much their surface emissions estimates are degraded by model error when using the SC approach.

p16 L15-18: I can not tell from Fig 12 and 13 that the high latitude a priori bias is smaller in 2x2.5 compared to 4x5. Similar question for the model bias reduction. It may just be that the color scale saturates so quickly in the images? Are they zonal avg summary stats you could provide to back this up?

p17 L10: "The results suggest that GEOS-Chem a priori CH4 simulation suffered from biases that were not related only to incorrect surface emissions." Since GEOS-Chem is not perfect (i.e. the real world has different transport) this is the most obvious source of the errors.

p18 L5: I find it a bit perplexing that 2x2.5 sims are generally argued to provide better atmospheric transport but perform more poorly against in situ obs, which one would think would be the most sensitive to things like vertical transport. Would you consider this an indication of residual error in surface CH4 fluxes?

Tables 1 & 2: These comparisons to independent data are powerful demonstrations that using the weak constraint approach on the GOSAT XCH4 data really does improve the estimated 3D CH4 fields better than the SC approach. Apparently either the transport or the measurements are bad enough that the WC results in a big improvement. If the GOSAT data are badly biased, adding flex in the state trajectory would help things, even if the transport were not too bad.

p22 L30: I get the averaging out of resolved eddy motions causing problems but what are you referring to by "incorrect" regridding?

p23 L28: "Despite having almost flat averaging kernels in the troposphere..." Show a plot of the GOSAT XCH4 averaging kernel – since GOSAT measures it in a thermal IR band, I would have thought that the averaging kernel would be mainly sensitive to the upper troposphere.

Minor Comments: p5 line 13: should this read "and the GHG_CCI group"??

p5 L20: "produced a comparable fit...": to what, the old three-model suite used in the

retrievals?

p5 L24: you should say GOSAT "XCH4" here, since that is what you are looking at; "CH4" does better than that, I think.

P21 L25-26: Reword these lines, I don't think the CH4 budget is conserved because there is bias in the stratosphere induced by transport error.

P23 l8: add a comma before "are"

In general, I would prefer full descriptions like "the difference between A and B" as opposed to the "bias in A". The term "bias" means a lot of different things, and can relative to another unspecified quantity, and using the full description is always going to be less confusing albeit more wordy.

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